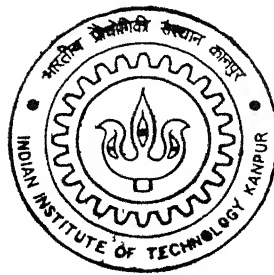


ESTIMATION OF UNSATURATED FLOW PARAMETERS FROM COLUMN OUTFLOW EXPERIMENT

By

Pankaj Kumar Saxena



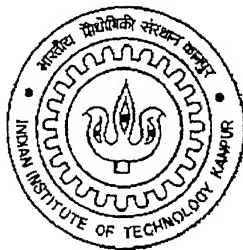
DEPARTMENT OF CIVIL ENGINEERING
Indian Institute of Technology Kanpur

AUGUST, 2002

ESTIMATION OF UNSATURATED FLOW PARAMETERS FROM COLUMN OUTFLOW EXPERIMENT

A Thesis submitted
In Partial Fulfillment of the Requirements
For the Degree of
MASTER OF TECHNOLOGY

by
PANKAJ KUMAR SAXENA



to the
DEPARTMENT OF CIVIL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY, KANPUR

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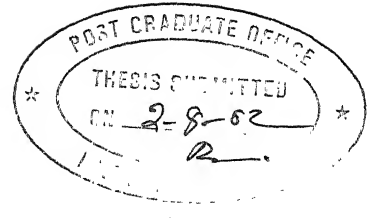
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CERTIFICATE

It is certified that the work presented in this thesis entitled "**Estimation of parameters by constant flux soil column**" by **Pankaj Kumar Saxena** , has been carried out under my supervision in partial fulfillment of the requirement for the award of M. Tech. degree in Civil Engineering. This thesis is a record of bonafide work carried out in the Department of Civil Engineering, I.I.T. Kanpur during the year 2001-2002 and this work has not submitted elsewhere for a degree.

August, 2002

A handwritten signature in black ink, appearing to read "Rajesh Srivastava".

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CONTENTS

CERTIFICATE	i
ACKNOWLEDGEMENTS	ii
CONTENTS	iii
LIST OF FIGURES	v
LIST OF SYMBOLS	vi
ABSTRACT	vii
CHAPTER 1: INTRODUCTION	1-6
1.1 GENERAL	1
1.2 TECHNIQUES TO DETERMINE RELATIONSHIP BETWEEN h , θ AND K	2
1.3 MATHEMATICAL MODELS AND RICHARD'S EQUATION	4
CHAPTER 2: OUTLINE OF PRESENT PROBLEM AND LITERATURE REVIEW	7-15
2.1 INTRODUCTION	7
2.2 PURPOSE OF PRESENT STUDY	9
2.3 VGM MODEL	10
2.3.1 Shape of hydraulic function	11
2.3.2 Values of parameters α and n	14
2.4 MODIFIED PICARD'S APPROXIMATION	15
CHAPTER 3: PROBLEM FORMULATION AND SIMULATION	16-22
3.1 GENERAL	16
3.2 SUITABILITY OF VARIOUS FORMS OF RICHARD'S EQUATION	17

3.3 FORMULATION	18
3.3.1 Discretisation of boundary condition	21
3.3.2 Estimating the inter-block hydraulic conductivity	21
3.4 NUMERICAL SIMULATION	22
CHAPTER 4: RESULTS AND DISCUSSION	23-36
4.1 OUTFLOW VS. TIME: EFFECT OF α AND n	23
4.2 VARIATION OF T_{50} AND S_{60-40}	27
4.3 RELATIONSHIP OF T_{50} AND S_{60-40} WITH PARAMETERS ...	32
4.3.1 Mathematical expression for parameters	32
4.3.2 Graphical representation of T_{50} and S_{60-40} to estimate parameters	34
CHAPTER 5: CONCLUSIONS AND FUTURE STUDY	37-38
5.1 CONCLUSIONS	32
5.2 RECOMMENDATIONS FOR FUTURE WORK.....	33
REFERENCES	39-44

LIST OF FIGURES

Fig. 2.1 Plot of θ vs. h for different values of n	12
Fig. 2.2 Plot of C vs. h	12
Fig. 2.3 Plot of K_r vs. h	13
Fig. 4.1 Pattern of outflow variation with n	23
Fig. 4.2 Pattern of outflow variation with α varying	24
Fig. 4.3 Pressure head distribution with varying n and keeping α constant.	26
Fig. 4.4 Pressure head distribution with varying α and keeping n constant.	26
Fig. 4.5 T_{50} vs. α , keeping constant value of $n = 2.0$	27
Fig. 4.6 T_{50} vs. n , keeping constant value of $\alpha = 0.04$	28
Fig. 4.7 S_{60-40} vs. α , keeping constant value of $n = 2.0$	30
Fig. 4.8 S_{60-40} vs. n , keeping constant value of $\alpha = 0.04$	30
Fig. 4.9 Error in α and n back-calculated from eq (4.9) & (4.14), for 252 data sets obtained from simulation	33
Fig. 4.10 S_{60-40} vs. T_{50} : graphical representation of studied domain of numerical values of parameters	34
Fig. 4.11 S_{60-40} vs. T_{50} plot at higher parameter values	35

LIST OF SYMBOLS

z	Datum head (+ve downward)
L	Height of soil column
t	time from start of flow
h	Pressure head
θ	Volumetric moisture content
θ_s	Saturated moisture content
θ_r	Residual moisture content
S_e	Effective saturation
K	Unsaturated hydraulic conductivity
K_s	Saturated hydraulic conductivity
K_r	Relative hydraulic conductivity
q	Darcy's flux
l	Pore connectivity parameter
α, m, n	VGM parameters
C	Moisture capacity
D	Unsaturated Diffusivity
VGM	van Genuchten – Mualem (model)
ODE	Ordinary differential equation
OS	One-step (outflow method)
MS	Multi-step (outflow method)

ABSTRACT

Accurate, reliable and efficient simulations of moisture fluxes through porous media are desirable in hydrological and environmental studies, as well as in civil and environmental engineering. For these simulations we need reliable estimate of flow parameters. Several mathematical models are available, which attempt to describe various soil-hydraulic parameters. Among these parameters, hydraulic conductivity K is the one, which still needs a serious attention. The most acceptable mathematical prediction of K is given by a model, originally proposed by Mualem and then modified by van Genuchten and hence known as VGM model. The correct prediction of K depends on the model parameters α and n and hence the suitable values of these parameters are required to be determined first. This dissertation is aimed at determination of suitable values of α and n from column outflow experiment. The outflow is simulated for a possible range of α and n and then by the analysis of these outflow patterns two quantities, namely, T_{50} and slope (S_{60-40}), have been found to have a coherent relationship with VGM parameters, hence, are suitable for calibration of these parameters. A graphical representation has been given from which value of α and n can be directly interpreted.

Chapter 1

INTRODUCTION

1.1 General

The desire and necessity to explore nature for our civilizational development ignites the zeal to understand the enigmatic style, in which water, one of the basic element of nature, behaves. Moreover, if the water is in form of groundwater, the phenomenon becomes highly erratic.

With increasing demands on groundwater resources the need for an accurate prediction of the subsurface flow and chemical species transport under different hydro-geological, climatic and ecological conditions have greatly accentuated the need to understand these processes and to evaluate effects of management practices and remediation techniques. Accurate, reliable and efficient simulations of moisture fluxes through porous media are desirable in hydrological and environmental studies, as well as in civil and environmental engineering. The ability to model time dependent flows in composite soil formations that may be intermittently saturated and drained is particularly important from the point of view of physical realism. Several computer codes based on numerical models have been used, but with these powerful tools, comes the need for the ability of accurate determination of required model parameters. In some cases, only groundwater flow is of interest, and the saturated hydraulic conductivity, K_s , must be

determined. However, the processes of flow and transport in the vadose zone are essential because most groundwater contaminant sources originate in this zone. Model calibration in the unsaturated zone may be particularly difficult due to problems in formulating the constitutive relations for this special type of two-phase flow, namely the water retention curve and the unsaturated hydraulic conductivity.

1.2 Techniques to determine relationship between h , θ and K

There are some laboratory and field methods to determine the relationships between the pressure head h , the water content θ , and the hydraulic conductivity K . Traditionally, direct steady-state methods for the determination of these highly non-linear functions exist [*Klute and Dirksen (1986)*], but recently, transient experimental methods coupled with inverse modelling techniques have become more attractive [*Kool et al (1987)*, *Yeh (1986)*]. This parameter identification technique involves the numerical solution of the water flow equation for unsaturated/saturated porous media, subject to the imposed initial and boundary conditions. The constitutive relations, the so-called hydraulic properties are assumed to be described by analytical functions characterized by a limited number of parameters. During an experiment some auxiliary variables are measured, e.g. cumulative outflow, pressure head, water content, or infiltration. Then, the priori unknown parameters are determined by minimizing the objective function containing the deviations between observed and predicted quantities.

The use of laboratory outflow experiments for estimation of unsaturated hydraulic properties is advantageous because it is flexible in initial and boundary conditions and

not very time-consuming. One-step outflow experiments (OS), where an initial saturated soil column is drained by a one-step pressure change at the lower boundary, were used in conjunction with inverse modelling techniques first by *Parker et al.* (1985) and *Kool et al* (1985). If only cumulative water outflow is measured there, the inverse problem could be ill-posed and lead to a non-unique solution [*Zurmuhl* (1996)]. Finally, it appears that either equilibrium data are needed [*Van Dam et al* (1992)], or measurements of pressure head at one point inside the soil column can improve the performance of the OS-method [*Toorman et al* (1992)]. However, OS methods on large columns can produce dynamic capillary pressure-saturation relationships depending on the lower boundary value changes [*Vachaud et al* (1972), *Stuffer* (1978), *Nutzmann et al* (1994)]. The reasons for that and a theoretical model of such relationships were discussed by *Hassanizadeh* (1997).

These considerations stimulated the investigation of the multi-step outflow method (MS), which uses small pressure steps to induce drainage of the soil column. Superiority of the MS to the OS-method on small columns was reported in *Van Dam et al* (1994). They showed that the MS experiments with only cumulative outflow data contain sufficient information for the unique determination of the soil hydraulic functions, using initial estimates derived from the outflow experiment itself. *Eching and Hopmans* (1993) found that the inverse solution technique is greatly improved when cumulative outflow data are supplemented with simultaneously measured pressure head data from some position inside the column during the MS-experiment.

To study the reason for this behaviour the mathematics of inverse problems has to be considered. *Carrera and Neuman* (1986) defined criteria of identifiability and

uniqueness according to which inverse problems are well-posed for determining the aquifer parameters of groundwater flow. *Russo et al* (1991) and *Toorman et al* (1992) analyzed conditions of well-posedness by evaluating the response surfaces of an inverse problem to estimate the unsaturated hydraulic properties. As shown by *Mous* (1993), the non-uniqueness of the estimates is not due to a bad choice of the optimization algorithm, but is merely a consequence of the structure of the model and the design of the experiment. Based on a rank-analysis of the Hessian matrix conditions of local identifiability could be proved, and the number of identifiable parameters related to the experiment was calculated. *Zurmuhl* (1996) investigated parameter identifiability and uniqueness on OS and MS experiments with respect to sensitivity coefficients, and showed that only the MS-method can produce uncorrelated and thus linear independent parameters.

One-step and multi-step experiments commonly were carried out on small in-situ soil samples. *Eching and Hopmans* (1993) pointed out that the optimized soil hydraulic functions as determined from soil cores do not necessarily represent in-situ soil behaviour. This may be due to the heterogeneity of undisturbed soil cores and their small sizes [*Kool and Parker* (1988)].

1.3 Mathematical models and Richard's equation

Mathematical models typically use the Richard's equation to describe variably saturated flows. It is defined by coupling a statement of flow continuity with the Darcy's equation and is commonly cast into one of the following forms:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[D(\theta) \frac{\partial \theta}{\partial z} \right] - \frac{\partial K(\theta)}{\partial z} \quad (\text{Moisture-based } \theta\text{-form}) \quad (1.1)$$

$$C(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[K(h) \frac{\partial h}{\partial z} \right] - \frac{\partial K(h)}{\partial z} \quad (\text{Pressure-based, } h\text{-form}) \quad (1.2)$$

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K(\theta) \frac{\partial h}{\partial z} \right] - \frac{\partial K(h)}{\partial z} \quad (\text{Mixed or coupled form}) \quad (1.3)$$

where h is the pressure head [L], $\theta(h)$ is the volumetric moisture content, t is time [T], z is the (positive downward) depth [L], $K(h)$ or $K(\theta)$ [L/T] is the unsaturated hydraulic conductivity, $C(h) = d\theta/dh$ [1/L] is the moisture capacity and $D(\theta) = K(\theta)/C(\theta)$ is unsaturated diffusivity [L²/T].

The solution of Richard's equation requires the specification of soil constitutive functions:

- Hydraulic conductivity $K(h)$ [L/T],
- Specific capacity $C(h) \equiv d\theta/dh$ [L⁻¹] and
- Diffusivity $D(\theta) \equiv K(\theta)/C(\theta)$ [L²/T].

The combination of highly non-linear constitutive functions with non-trivial boundary and initial conditions precludes all but the most simplified analytic approaches to the solution of (1.1), (1.2) and (1.3). Common practical approaches for the analysis of variably saturated flows are mixed and pressure-based numerical formulations, which employ low-order finite difference or finite element spatial discretisation and simple Euler time stepping [Celia *et al* (1990), Paniconi *et al* (1991), Rathfelder and Abriola

(1994), *Bergamaschi and Putti et al* (1999)]. The numerical stability of the temporal approximation is enforced by employing implicit (typically, backward Euler) time stepping, while oscillations in the finite element spatial discretisation are controlled by lumping [*Celia et al* (1990), *Ju and Kung* (1997)]. Substantial research has also been dedicated to the solution of the non-linear discrete systems that arise in implicit time stepping schemes [*Paniconi et. al.* (1991), *Lehmann and Ackerer* (1998), *Miller et al* (1998)], and to the incorporation of the soil constitutive relationships [*Miller et al* (1998)].

An appreciable advantage of a numerical scheme based on the mixed form of Richard's equation is its inherent conservation of mass. Conversely, standard numerical approximations based on the pressure form of Richard's equation develop undesirable mass balance problems [*Celia et. al.* (1990)], seriously undermining their physical basis.

In practical applications where the computational speed of the solution is an important priority, numerical errors of the order of 0.1-1% are typically acceptable. In these cases low-order schemes are competitive with higher-order solvers, and may in fact be preferred due to their better stability and algorithmic simplicity [*Wood* (1990)]. Numerical experiments have shown, for example, that the second-order accurate Crank-Nicolson scheme outperformed the first-order accurate backward Euler scheme only when relative errors below 0.005% were required [*Wood* (1990)]. The results of other numerical investigations [e.g., *Paniconi et. al.* (1991) and *Tocci et. al.* (1997)] also suggest that low-order schemes are competitive with higher-order schemes when coarse time steps are used. Indeed, most practical codes implement simple first- or second-order approximations [*Celia et al* (1990)].

Chapter 2

OUTLINE OF PRESENT PROBLEM AND LITERATURE REVIEW

2.1 Introduction

For 1-D vertical flow, Richard's equation is given by:

$$\frac{\partial \theta(h)}{\partial t} = \frac{\partial}{\partial z} \left[K(h) \frac{\partial h}{\partial z} - K(h) \right] \quad (2.1)$$

Water movement through the unsaturated zone is commonly analyzed by solving Richard's equation [Richards (1931)]. Analytical and simplified solutions of Richard's equation [Philip (1969), Parlange (1972), Broadbridge et al (1988), Warrick (1991)] provide useful tools for studying simple unsaturated flow systems with relatively simple initial and boundary conditions. The solutions of these models are based on the following assumptions:

- (i) Soil is homogeneous,
- (ii) Initial moisture content is uniform throughout the soil profile, and
- (iii) Moisture content at the soil surface is constant and rainfall or irrigation rate is constant.

In addition, models give accurate results only for a particular type of soil. For example, Green-Ampt Model, which is based on the assumption of saturated plug flow, fails in situations where a coarse textured soil with high hydraulic conductivity underlies

a fine textured soil with low hydraulic conductivity [*Chow* (1988)]. In the field, soils are seldom homogeneous, initial moisture content is seldom uniformly distributed and in most field situations during rainfall or irrigation, the soil surface is rarely at constant saturation. For accurate prediction of moisture movement under realistic boundary conditions in field soils, one has to resort to numerical models, which are versatile in handling the non-homogeneity and different kinds of boundary conditions.

Then comes the measurement of the unsaturated conductivity. Accurate measurement is generally cumbersome, costly, and very time-consuming. Consequently, many attempts have been made to develop indirect methods that predict the conductivity function from the more easily measured water retention curve [*Mualem* (1976), *Leij* (1996)]. Most of the predictive conductivity models are based on the assumption of having an ideal capillary medium characterized by a certain pore-size distribution function. Although not necessarily valid for all soils, this assumption is widely accepted as an effective working hypothesis [*Mualem* (1976)].

A variety of empirical equations have been used to describe the soil water retention curve. One of the most popular equations is the power-law function initially proposed by *Brooks and Corey* (1964). This equation leads to an air-entry value, h_a , in the soil water retention curve above which the soil is assumed to be saturated. The Brooks and Corey equation was modified by *van Genuchten* (1980) to enable a more accurate description of observed soil hydraulic data near saturation, especially for undisturbed and many fine-textured soils. The choice of the analytical model for $\theta(h)$ can significantly affect the predicted $K(h)$ function obtained with one of the statistical pore-size distribution models. One reason for this is that the predicted conductivity function is

extremely sensitive to small changes in the *shape* of the retention curve near saturation [Vogel *et. al.* (2001)]. This sensitivity is a major cause of the sometimes significant differences between predicted $K(h)$ functions obtained with the Brooks and Corey and van Genuchten retention functions. The differences are specially important for fine-textured soils which can exhibit extreme non-linearity in $K(h)$ close to saturation when Van Genuchten's equations are used. The differences are generally much less severe for coarse-textured soils.

The presence of highly non-linear $K(h)$ relationships near saturation can also substantially impact the performance of numerical solutions of Eq. (2.1) in terms of the accuracy, stability, and rate of convergence of the invoked numerical scheme [Vogel *et. al.* (2001)]. While numerical solutions for solving the variably saturated flow equation have been significantly improved in recent years [Milly (1985), Celia *et. al.* (1990), Kirkland *et. al.* (1992), Huang *et. al.* (1996)], most improvements focused on numerical problems associated with the infiltration of water in very dry coarse-textured soils [hills *et. al.* (1989), Huang *et. al.* (1996)].

2.2 Purpose of present study

Several numerical models have been developed for simulating water movement in unsaturated porous media using finite difference, finite element, and integrated finite difference methods. Most of the numerical models considered focus their attention either on improving the existing methods or on concentrating on one process such as infiltration, gravity drainage or evaporation. However, very few attempts have been made

to study the sensitivity of different processes with respect to the unsaturated soil parameters. The objective of the present study is

- to analyze VGM model and study the effect of model parameters (α and n) on 1-D transient flow in vadose zone.
- To develop a methodology for identification of the VDM parameters for given outflow data.

2.3 VGM Model

The predictive model of Mualem (1976) for the relative hydraulic conductivity function, $K_r(h)$, may be written in the form:

$$K_r(S_e) = S_e^l \left[\int_0^{S_e} \frac{dx}{h(x)} \right]^2 \bigg/ \left[\int_0^1 \frac{dx}{h(x)} \right]^2 \quad (2.2)$$

where $K_r = K/K_s$, K is the unsaturated hydraulic conductivity, K_s the saturated hydraulic conductivity, l the pore connectivity parameter usually assumed to be 0.5 following Mualem (1976), and S_e is the effective saturation given by

$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} \quad (2.3)$$

where $\theta(h)$ is the volumetric water content, and θ_r and θ_s are the residual and saturated water contents, respectively. Substituting van Genuchten's (1980) expression for the soil water retention curve, i.e.,

$$\theta(h) = \begin{cases} \theta_r + \frac{\theta_s - \theta_r}{[1 + (\alpha \cdot h)^n]^m} & h < 0 \\ \theta_s & h \geq 0 \end{cases} \quad (2.4)$$

into Eq. (2.2) leads to the following equation for the unsaturated hydraulic conductivity

$$K(h) = \begin{cases} K_s K_r(h), & h < 0 \\ K_s, & h \geq 0 \end{cases} \quad (2.5)$$

where

$$K_r(S_e) = S_e' \left[1 - (1 - S_e'^{1/m})^m \right]^2 \quad (2.6)$$

in which n and α are empirical shape parameters (with $n > 1$), and $m = 1 - 1/n$. The restriction $m = 1 - 1/n$ is necessary to permit direct integration of Eq. (2.2) once the inverse of Eq. (2.4) is substituted into Eq. (2.2). Much more complicated expressions for $K_r(h)$ result when the parameters m and n are assumed to be mutually independent [Vogel *et al* (2001)]. In this dissertation, Eqs. (2.4) to (2.6) will be referred as the VGM model.

2.3.1 Shape of hydraulic function

Now let us see how VGM equations describe the soil hydraulic functions. Fig. (2.1) to (2.3) show variations in the soil hydraulic characteristics for a series of n -values, while keeping all other parameters constant ($\alpha = 0.005 \text{ cm}^{-1}$, $\theta_s = 0.40$ and $\theta_r = 0.10$).

Notice that the $K_r(h)$ function in Fig.2.3 exhibits an abrupt drop at saturation when n becomes less than about 1.5. The magnitude of the decrease at $h = 0$ depends not only on the parameter n , but to a lesser extent also on α , which may be viewed as a scaling factor for h . The extreme non-linearity occurs only when $1 < n < 2$. Close inspection of Fig. (2.2) and (2.3) shows that the soil water capacity function, $C(h)=d\theta/dh$, and relative

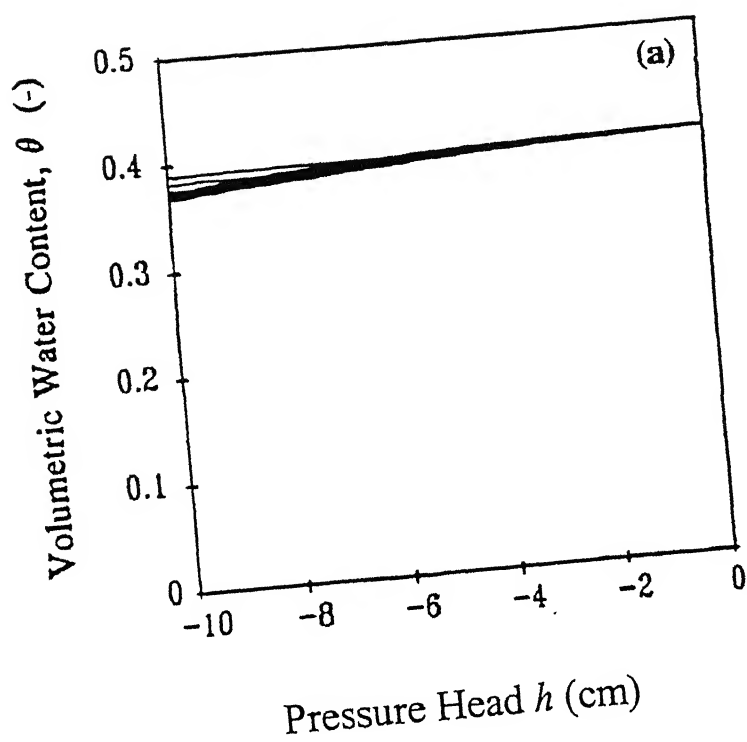


Fig. 2.1 Plot of θ vs. h for different values of n

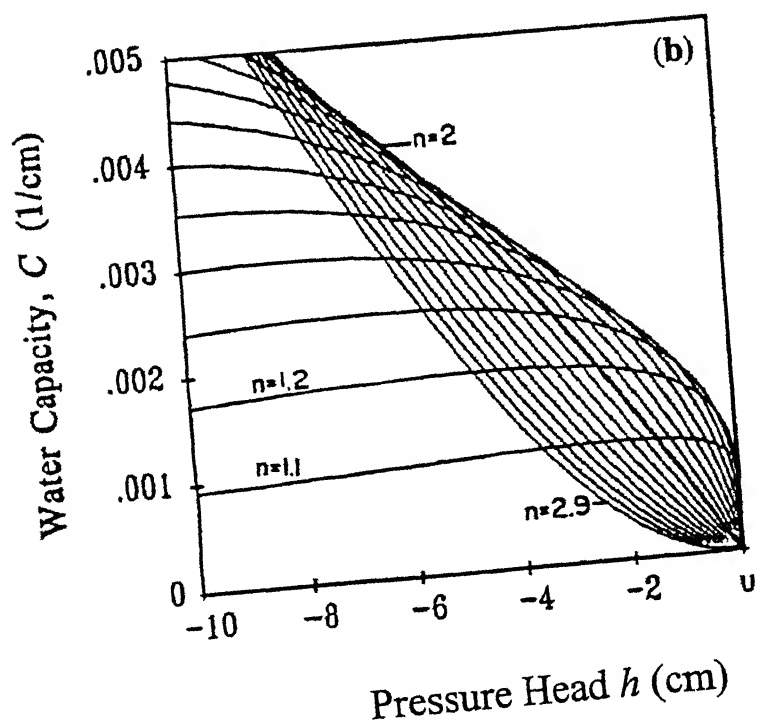


Fig. 2.2 Plot of C vs. h

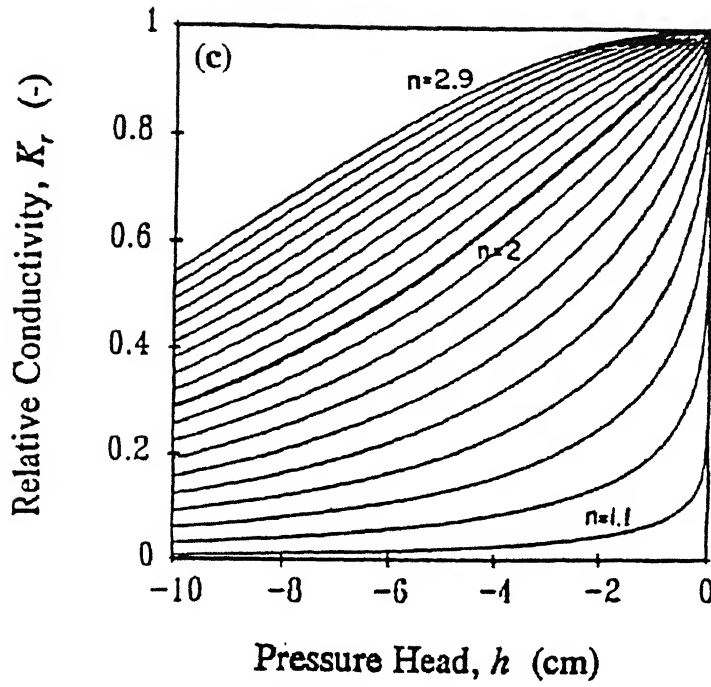


Fig. 2.3 Plot of K_r vs. h

conductivity function, $K_r(h)$, both change their shape near saturation when n changes from $n < 2$ to $n > 2$. Vogel *et al* (2001) has discussed that the slopes of these two functions change from $-\infty$ for $C(h)$ and ∞ for $K_r(h)$ when $n < 2$ to some non-zero finite values when $n = 2$, and to zero when $n > 2$. This effect of the value of n on the shape of the retention curve near saturation was discussed previously by Luckner *et al* (1989). They showed that the restriction $n > 1$ guarantees only first-order continuity in $\theta(h)$ at saturation, while $n > 2$ ensures also second-order continuity in $\theta(h)$, and hence first-order continuity in $C(h)$.

2.3.2 Values of parameters α and n

As the soil properties tend more towards sand, the value of α and n increases. Average values of VGM soil hydraulic parameters for 12 major soil textural groups, according to *Carsel and Parrish* (1988) are given below:

Table 2.1:

Texture	θ_r (m ³ /m ³)	θ_s (m ³ /m ³)	α (cm ⁻¹)	n	K_s (cm/day)
(1) Sand	0.045	0.430	0.145	2.68	712.80
(2) Loamy sand	0.057	0.410	0.124	2.28	350.20
(3) Sandy Loam	0.065	0.410	0.075	1.89	106.10
(4) Loam	0.078	0.430	0.036	1.56	24.96
(5) Silt	0.034	0.460	0.016	1.37	6.00
(6) Silt loam	0.067	0.450	0.020	1.41	10.8
(7) Sandy clay loam	0.10	0.390	0.059	1.48	31.44
(8) Clay loam	0.095	0.410	0.019	1.31	6.14
(9) Silty clay loam	0.089	0.430	0.010	1.23	1.68
(10) Sandy clay	0.100	0.380	0.027	1.23	2.88
(11) Silty clay	0.070	0.360	0.005	1.09	0.48
(12) Clay	0.068	0.380	0.008	1.09	4.80

2.4 Modified Picard (chord slope) approximation:

The classic method of Celia *et. al.* (1990) is based on a backward difference approximation to $d\theta/dt$ in first order ODE system:

$$M \frac{d\theta}{dt} + K h = F \quad (2.7)$$

$$M^{n+1} \frac{\theta^{n+1} - \theta^n}{\Delta t} + K^{n+1} \Psi^{n+1} + F^{n+1} \quad (2.8)$$

This non-linear system can be solved using a modified fixed-point (modified Picard) iteration:

$$[C^{n+1,m} + \Delta t K^{n+1,m}] \delta h^{m+1} = -\{\Delta t (F^{n+1,m} + K^{n+1,m} h^{n+1,m}) + M^{n+1,m} (\theta^{n+1,m} - \theta^n)\}, \quad (2.9)$$

$$h^{n+1,m+1} = h^{n+1,m} + \delta h^{m+1}. \quad (2.10)$$

(2.9) and (2.10) will be referred to as the Celia *et al.* solution to Richards equation. In the Celia *et al.* scheme, $d\theta/dh$ in the C matrix is evaluated analytically. Rathfelder and Abriola (1994) showed that the Celia *et al.* scheme is equivalent to a pressure-based backward Euler formulation, with the specific capacity $d\theta/dh$ approximated using a chord-slope estimate:

$$\left(\frac{d\theta}{dh}\right)^{n+1} \cong \frac{\Delta\theta}{\Delta h} = \frac{\theta^{n+1} - \theta^n}{h^{n+1} - h^n} \quad (2.11)$$

This approximation, proposed by Celia *et al* (1990), has been used in formulation of flow in present study, which has been discussed in chapter 3.

Chapter 3

PROBLEM FORMULATION AND SIMULATION

3.1 General

The whole study in this dissertation is aimed at removing the cumbersome numerical procedure and difficult experimental data, for the identification of VGM parameters for different soils. Presently, most of the available methods are based on head-measurement and those, which are based on outflow, too require pressure head at some location of soil column.

As for as experimental convenience is concerned, head-measurement requires sophisticated transducers and other accessories to maintain the required precision of experimental data. On the other hand, discharge measurement is comparatively simple process and data can be easily obtained.

So, the objective is to calibrate the VGM parameters and develop a procedure for which the only information to be supplied, is outflow of soil column. This will enable us to extract suitable values of VGM parameters more easily, to simulate the unsaturated flow mathematically.

The work of this dissertation have been done in two steps:

1. Simulation of VGM outflow for possible range of α and n .
2. Analysis of various data sets obtained from previous step.

Above two steps have been resulted in the shape of equations from which the parameters can be calculated by extracting two factors, namely, T_{50} and S_{60-40} , from given outflow data. These factors will be discussed in detail in the section 3.4.1.

Before starting the discussion on outflow data, it is important to discuss the various forms of Richard's equation and their applicability.

3.2 Suitability of various forms of Richard's equation

Three forms of Richard's Equation as given in chapter1, can be written as below:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[D(\theta) \frac{\partial \theta}{\partial z} \right] - \frac{\partial K(\theta)}{\partial z} \quad (\text{Moisture-based } \theta\text{-form}) \quad (3.1)$$

$$C(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[K(h) \frac{\partial h}{\partial z} \right] - \frac{\partial K(h)}{\partial z} \quad (\text{Pressure-based, } h\text{-form}) \quad (3.2)$$

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K(\theta) \frac{\partial h}{\partial z} \right] - \frac{\partial K(h)}{\partial z} \quad (\text{Mixed or Coupled form}) \quad (3.3)$$

The terms on left side of above equations describe the effects of draining and filling pores, so statement in terms of the temporal change in moisture content is more appropriate than description via pressure. In other words, the term $(d\theta/dh)\partial h/\partial t$ is more appropriately written in its simpler form $\partial \theta/\partial t$.

On the right side of equations, it is noted that the spatial derivative of the hydraulic head is used to describe the driving force for fluid movement. This is the most direct mathematical statement of the fact that head differences do indeed supply the energy required to move fluid. Specification of hydraulic conductivity as a function of the

pressure head, $K(h)$, is, however, not directly representative of underlying physics. It is water-filled pores which facilitate transmission of water through the porous medium. Although, water content and pressure are directly related but formally, the hydraulic conductivity should be expressed in terms of the moisture content, $K(\theta)$. Besides, $K(h)$ typically exhibits hysteresis, where as in $K(\theta)$ this phenomenon is generally less pronounced [Nielsen (1986)].

Hence, the most direct mathematical expression of the physics of unsaturated flow, given the consideration above, is the mixed form presented in equation (3.3).

The present study, as explained earlier, intend to deal with discharge outflow and hence the boundary condition, considered here, is of Neumann type (constant flux) Boundary Condition, i.e.,

$$\begin{cases} h(z,0) = h_{initial}, & 0 < z < L \\ h(0,0) = h_0, \\ h(L,t) = h_{initial}, & t > 0 \\ q(0,t) = q_0, & t > 0 \end{cases}$$

3.3 Formulation

As discussed in chapter 1, finite difference scheme is used in present study. The standard finite difference method (FDM) for mixed form of Richard's equation obtained by a backward Euler method for temporal discretisation is

$$\frac{\theta_i^{n+1,m+1} - \theta_i^n}{\Delta t} = \frac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2} [h_{i+1}^{n+1,m+1} - h_i^{n+1,m+1}] + \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2} [h_i^{n+1,m+1} - h_{i-1}^{n+1,m+1}] + \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} \quad (3.4)$$

where $K_{i+1/2}^{n+1,m}$ indicate the inter-block hydraulic conductivities. The key to the method is expansion of $\theta_i^{n+1,m+1}$ in a truncated Taylor series with respect to h , about the expansion point $h_i^{n+1,m}$, namely,

$$\theta_i^{n+1,m+1} = \theta_i^{n+1,m} + \frac{d\theta}{dh} \bigg|^{n+1,m} (h^{n+1,m+1} - h^{n+1,m}) + O(\delta^2) \quad (3.5)$$

If all terms higher than linear are neglected in eq. (3.5) and it substituted into eq.(3.4), it results

$$\begin{aligned} \frac{C_i^{n+1,m}}{\Delta t} \delta_i^{n+1,m} + \frac{\theta_i^{n+1,m+1} - \theta_i^n}{\Delta t} &= \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2} (h_i^{n+1,m+1} - h_{i-1}^{n+1,m+1}) + \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2} (h_{i+1}^{n+1,m+1} - h_i^{n+1,m+1}) \\ &\quad - \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} \end{aligned} \quad (3.6)$$

Substituting the increment of pressure head at subsequent iteration levels, i.e.,

$$\delta_i^m = (h_i^{n+1,m+1} - h_i^{n+1,m})$$

from eq. (3.6), we get

$$\begin{aligned} C_i^{n+1,m} \frac{\delta_i^{n+1,m}}{\Delta t} - \left[\frac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2} (\delta_{i+1}^m - \delta_i^m) - \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2} (\delta_i^m - \delta_{i-1}^m) \right] &= \frac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2} (h_{i+1}^{n+1,m} - h_i^{n+1,m}) \\ - \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2} (h_i^{n+1,m} - h_{i-1}^{n+1,m}) + \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} - \frac{\theta_i^{n+1,m} - \theta_i^n}{\Delta t} &\equiv R_i^{n+1,m} \end{aligned} \quad (3.7)$$

where $R_i^{n+1,m}$ is defined as the residual associated with the *modified Picard iteration* [Celia *et al*, (1990)].

Now these equations (3.7) can be written in matrix form as

$$\begin{bmatrix}
 P_1^m & Q_1^m & 0 & 0 & 0 & \gg & \gg & 0 & 0 & 0 \\
 O_2^m & P_2^m & Q_2^m & 0 & 0 & \gg & \gg & 0 & 0 & 0 \\
 0 & O_3^m & P_3^m & Q_3^m & 0 & \gg & \gg & 0 & 0 & 0 \\
 0 & 0 & O_4^m & P_4^m & Q_4^m & \gg & \gg & 0 & 0 & 0 \\
 0 & 0 & 0 & O_5^m & P_5^m & \gg & \gg & 0 & 0 & 0 \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \gg & \vdots & \vdots & \vdots \\
 \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
 0 & 0 & 0 & 0 & 0 & \gg & \gg & P_{N-2}^m & Q_{N-2}^m & 0 \\
 0 & 0 & 0 & 0 & 0 & \gg & \gg & O_{N-1}^m & P_{N-1}^m & Q_{N-1}^m \\
 0 & 0 & 0 & 0 & 0 & \gg & \gg & 0 & O_N^m & P_N^m
 \end{bmatrix}
 \begin{bmatrix}
 \delta_1^m \\
 \delta_2^m \\
 \delta_3^m \\
 \delta_4^m \\
 \delta_5^m \\
 \vdots \\
 \vdots \\
 \vdots \\
 \delta_{N-2}^m \\
 \delta_{N-1}^m \\
 \delta_N^m
 \end{bmatrix}
 =
 \begin{bmatrix}
 R_1^m \\
 R_2^m \\
 R_3^m \\
 R_4^m \\
 R_5^m \\
 \vdots \\
 \vdots \\
 \vdots \\
 R_{N-2}^m \\
 R_{N-1}^m \\
 R_N^m
 \end{bmatrix} \quad (3.8)$$

where the coefficients O , P , Q and R are:

$$O_i^{n+1,m} = -\frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2};$$

$$P_i^{n+1,m} = \frac{C_i^{n+1,m}}{\Delta t} + \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2} + \frac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2};$$

$$Q_i^{n+1,m} = -\frac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2} \text{ and}$$

$$\begin{aligned}
 R_i^{n+1,m} = & \frac{K_{i+1/2}^{n+1,m}}{(\Delta z)^2} (h_{i+1}^{n+1,m} - h_i^{n+1,m}) - \frac{K_{i-1/2}^{n+1,m}}{(\Delta z)^2} (h_i^{n+1,m} - h_{i-1}^{n+1,m}) + \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} \\
 & - \frac{\theta_i^{n+1,m} - \theta_i^n}{\Delta t}
 \end{aligned}$$

3.3.1 Discretisation of boundary condition

In order to apply the boundary conditions eq. (3.8) is modified at the top and bottom node. In present study, Neumann type of boundary condition is applied, where flux is known at top node. It is given by

$$q = - \left[K \frac{\partial h}{\partial z} + K \right] \quad (3.9)$$

where q is the prescribed flux.

3.3.2 Estimating the inter-block hydraulic conductivity

The application of FDM provokes the problem of approximating the $i \pm 1/2$ label in space, referred to as “weighting” necessary for the determination of interblock hydraulic conductivity values $K_{i \pm 1/2}$. Different weighting formulas for estimating interblock quantities from the available grid point are proposed (Havekamp and Vauclin (1979).

Arithmetic mean

$$K_{i \pm 1/2} = \frac{K_i + K_{i \pm 1}}{2}$$

Geometric mean

$$K_{i \pm 1/2} = \sqrt{K_i K_{i \pm 1}}$$

Harmonic mean

$$K_{i \pm 1/2} = \frac{2K_i K_{i \pm 1}}{K_i + K_{i \pm 1}}$$

Upstream method

$$\begin{cases} K_{\pm 1/2} = K_{i \pm 1/2} & \text{if } h_{i \pm 1} > h_i \\ K_{\pm 1/2} = K_i & \text{if } h_{i \pm 1} < h_i \end{cases}$$

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Srivastava and Guzman (1995) has analyzed various formulas and recommended the use of geometric mean. In present analysis, the Richard's equation is approximated through modified Picard's scheme and solved with finite difference method. Geometric mean is used to carry out the inter-block hydraulic conductivity ($K_{i+1/2}$ and $K_{i-1/2}$).

3.4 Numerical simulation

for the numerical simulation all the quantities are considered in dimensionless form as follows:

$$h^* = h / L$$

$$\alpha^* = \alpha \cdot L$$

$$K^* = K / K_s$$

$$q^* = q / K_s$$

$$\theta^* = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

$$t^* = \frac{t \cdot K_s}{L \cdot (\theta_s - \theta_r)}$$

- Total depth of soil column $L = 100\text{cm}$
- Constant Darcy's flux at top $q_{\text{top}} = 0.5 K_s$

In the present study, the range of α is taken from 0.02 to 0.15 cm^{-1} and that of n is taken from 1.4 to 3.0.

Chapter 4

RESULTS AND DISCUSSION

4.1 Outflow vs. Time: Effect of α and n

Figure 3.1 and 3.2 shows pattern of outflow variation when n and α has been varied respectively, keeping all other factors constant.

Now, by observing the trends of these graphs, it can be easily noticed that the variation in the outflow, can mainly be described by two factors, namely

1. The time when the change in outflow occurs.
2. How rapid the outflow is increasing at saturation.

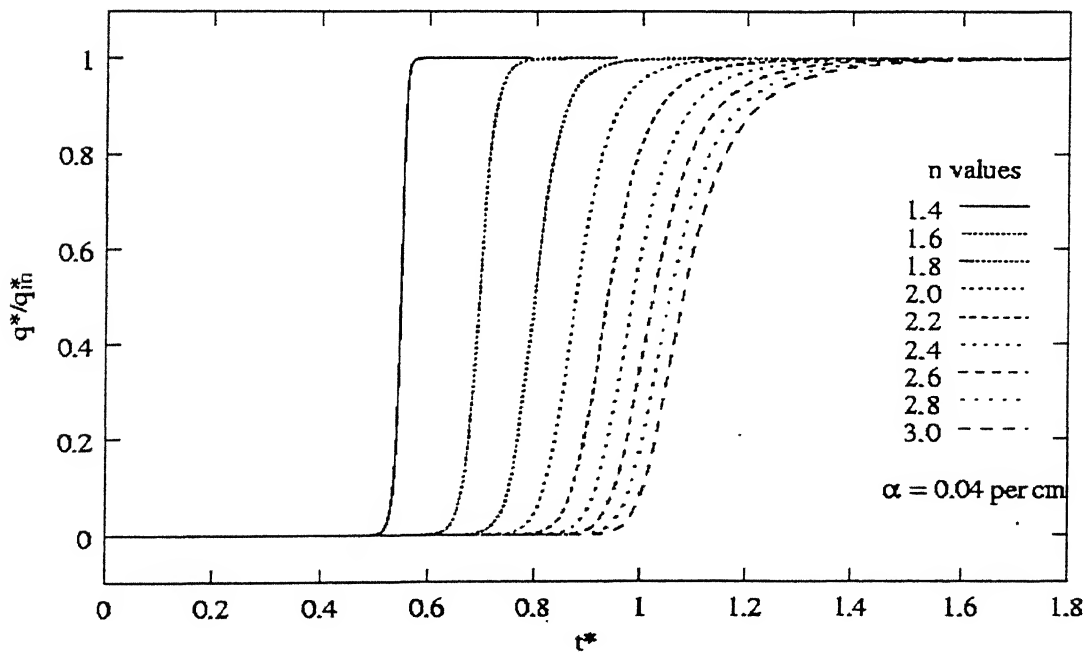


Fig. 4.1: Pattern of outflow variation with n .

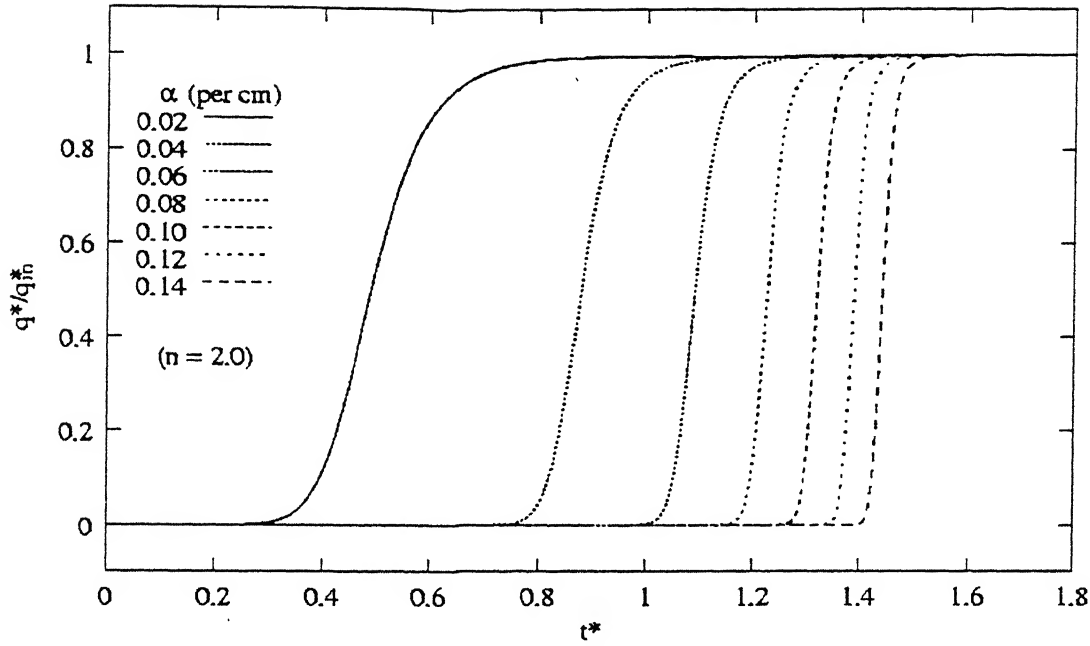


Fig. 4.2: Pattern of outflow variation with α varying.

Defining two quantities, T_{50} and S_{60-40} , as follows, can mathematically, represent the above two factors.

Time as T_{50} :

It is the time when outflow becomes 50% of the constant inflow at the top of soil column. As the graph shifts towards right, T_{50} will increase. Indeed, the time factor can be analysed by any T , not necessarily T_{50} . Still, T_{50} is better choice and this can be explained by the fact that for the estimation of parameters experimental data has to be used and hence the input (i.e., T) may have significant errors as it approaches to saturation. Error will also be dominating at the points where the outflow just starts increasing. In other words, the curved part of outflow may result in much higher degree of errors. Therefore, the best option is to be at comparatively straighter middle part. Thus T_{50} is a better choice of input data.

Slope as S_{60-40} :

It is clear from the above graphs that the slope of curve is not constant. In any outflow curve for some particular value of α and n first the slope is increasing from zero to some particular value S and then again decreasing to zero. This maximum value of slope, i.e., S is of interest as it is varying smoothly with α and n . The slope thus described can be represented as the difference of time T for two particular values of outflow:

$$S_{60-40} = T_{60} - T_{40} \quad (4.1)$$

where T_{60} and T_{40} are defined in the same fashion as T_{50} .

Again a lot of choices of T , are there. As it has been explained earlier that curved part should be avoided, but here the interesting aspect is that the difference must be large enough to overshadow the possible error in the experimental data. After analyzing various combinations slope defined in eq. (4.1) has been found to be the better choice.

FDM equations discussed in Section 3.3, have been simulated in dimensionless form, therefore, making T_{50} and S_{60-40} a dimensionless quantity. In the next step of present work, these two quantities have been studied and used for determining the VGM parameters.

Since the objective of this study is to estimate the parameters from outflow, only the outflow has been studied, but similar trends can be noticed in the pressure head. Figure 3.3 and 3.4 show the pressure head distribution at steady state for changing values of α and n .

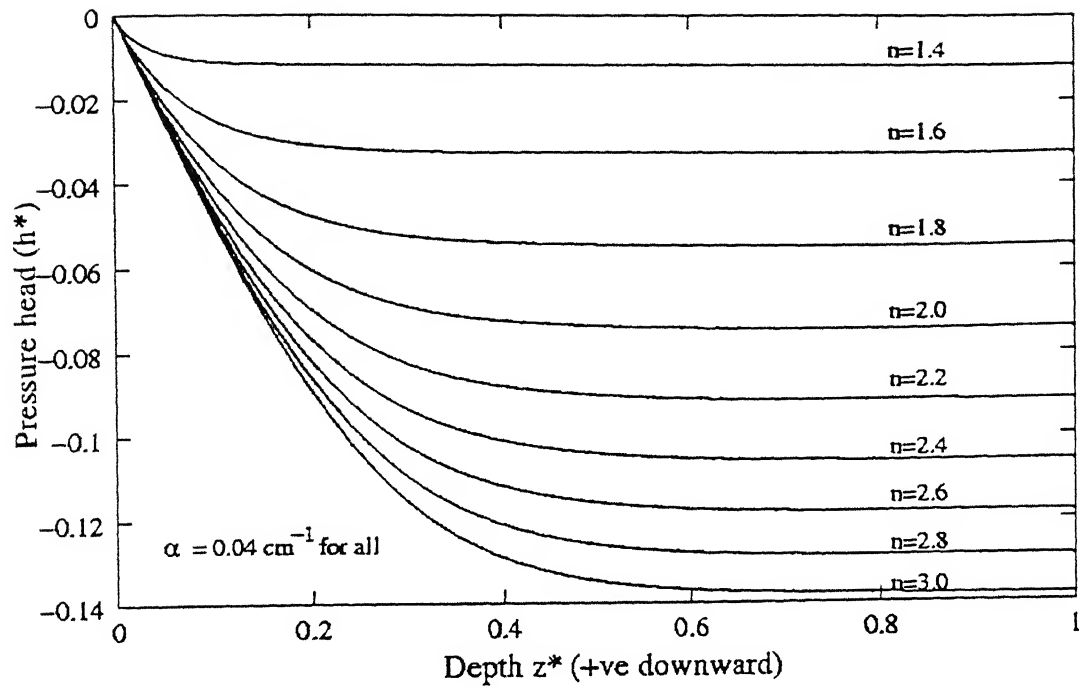


Fig. 4.3: Pressure head distribution with varying n and keeping α constant.

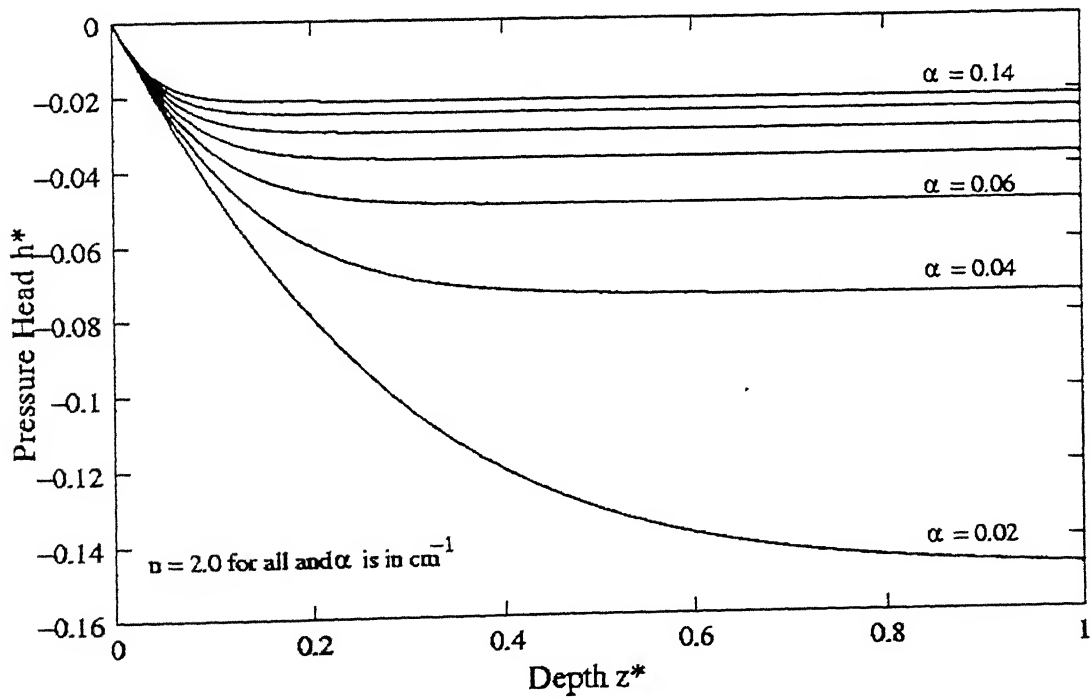


Fig. 4.4: Pressure head distribution with varying α and keeping n constant.

4.2 Variation of T_{50} and S_{60-40}

Fig (4.5) and (4.6) shows the pattern of T_{50} with respect to α and n respectively. It is very clear from the graphs that T_{50} is increasing with both α and n . the sensitivity of T_{50} is more w. r. t. α but in fig 4.5, as n increases the sensitivity is decreasing.

The curves obtained in fig 4.5, has been fitted in mathematical expression given in eq. (4.2) in order to obtain T_{50} , if the two parameters are known.

$$T_{50} = a \cdot (1 - e^{-b\alpha}) \quad (4.2)$$

where coefficients a and b , both are dependent of n .

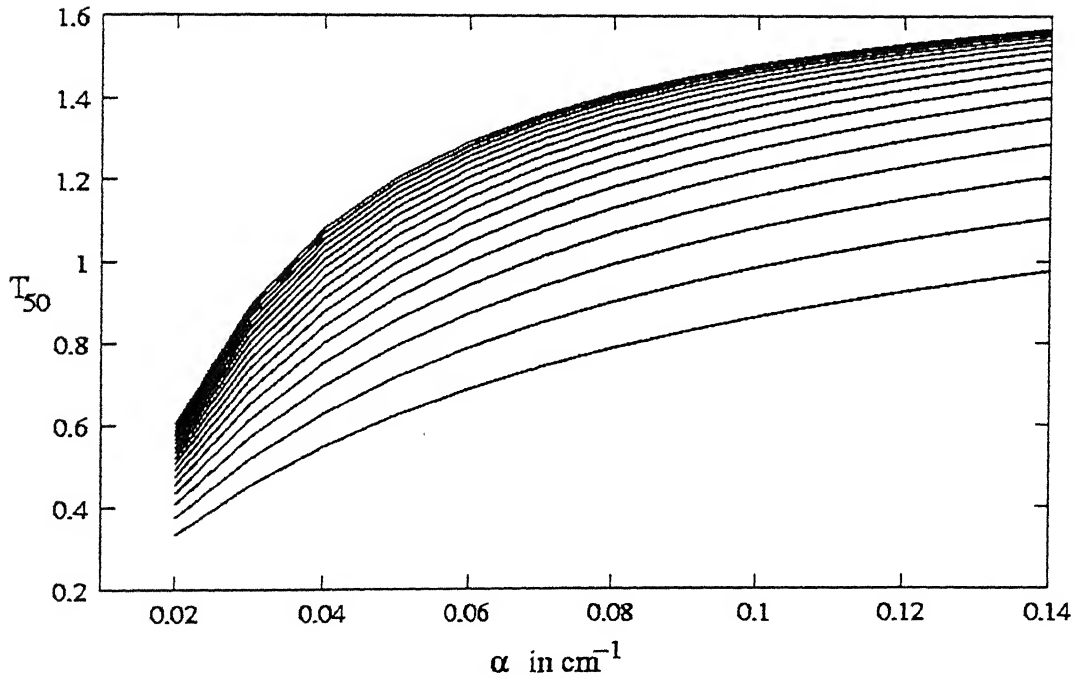


Fig. 4.5: variation of T_{50} with α

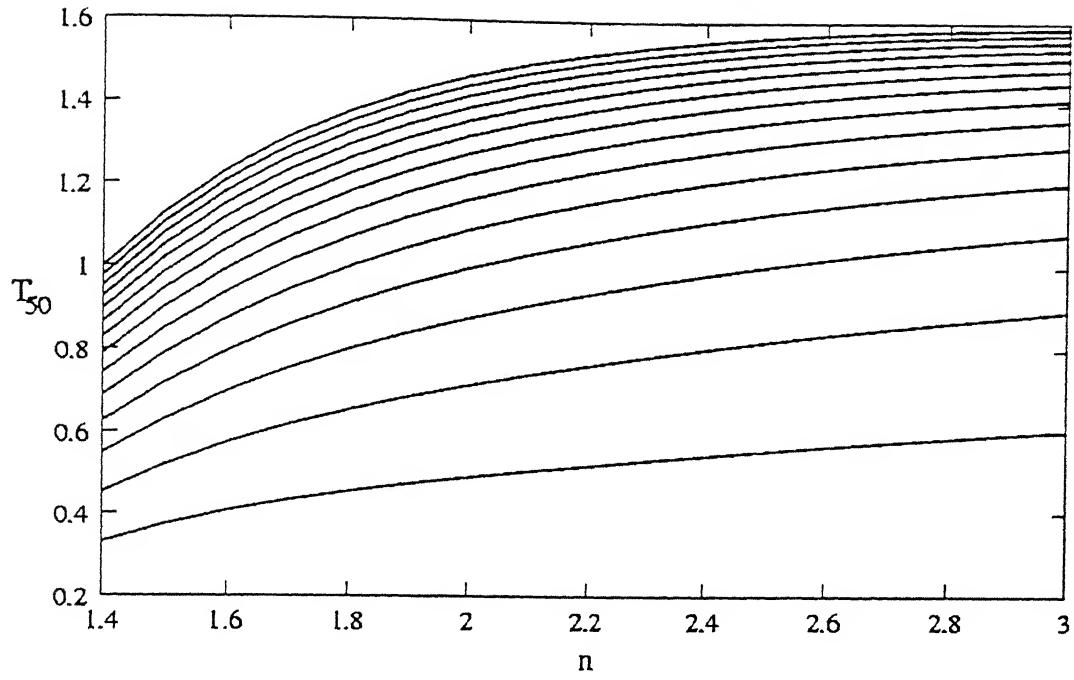


Fig. 4.6: variation of T_{50} with n

Various values of coefficients of eq. (4.2) are given below in Table 4.1.

Table 4.1 Values of coefficients of eq. (4.2) for different n

n	a	B
1.4	1.05069	17.93729
1.5	1.18563	18.40056
1.6	1.2902	18.86338
1.7	1.37096	19.34075
1.8	1.43307	19.84663
1.9	1.48047	20.38249
2.0	1.51634	20.9446
2.1	1.54333	21.52271
2.2	1.56343	22.11226

2.3	1.57817	22.70734
2.4	1.58877	23.3024
2.5	1.59616	23.89382
2.6	1.60103	24.47887
2.7	1.60395	25.05784
2.8	1.60533	25.6258
2.9	1.60557	26.18049
3.0	1.60489	26.72085

Again, these coefficients are fitted in polynomial models given by following equations

$$a = -\frac{1.2355}{\left(1 + \frac{n}{1.36362}\right)^{6.2945}} + 1.61946 \quad (4.3)$$

and

$$b = 9.85517 + 5.6091 \cdot n \quad (4.4)$$

Now, eq. (4.2)-(4.4) can give the value of T_{50} for any value of α and n

Similarly, the expression is also obtained for S_{60-40} . Fig (4.7) and (4.8) shows the pattern of S_{60-40} with respect to α and n respectively. Here, the point to be noticed is that the slope increases with increasing n , but decreasing with an increase in α .

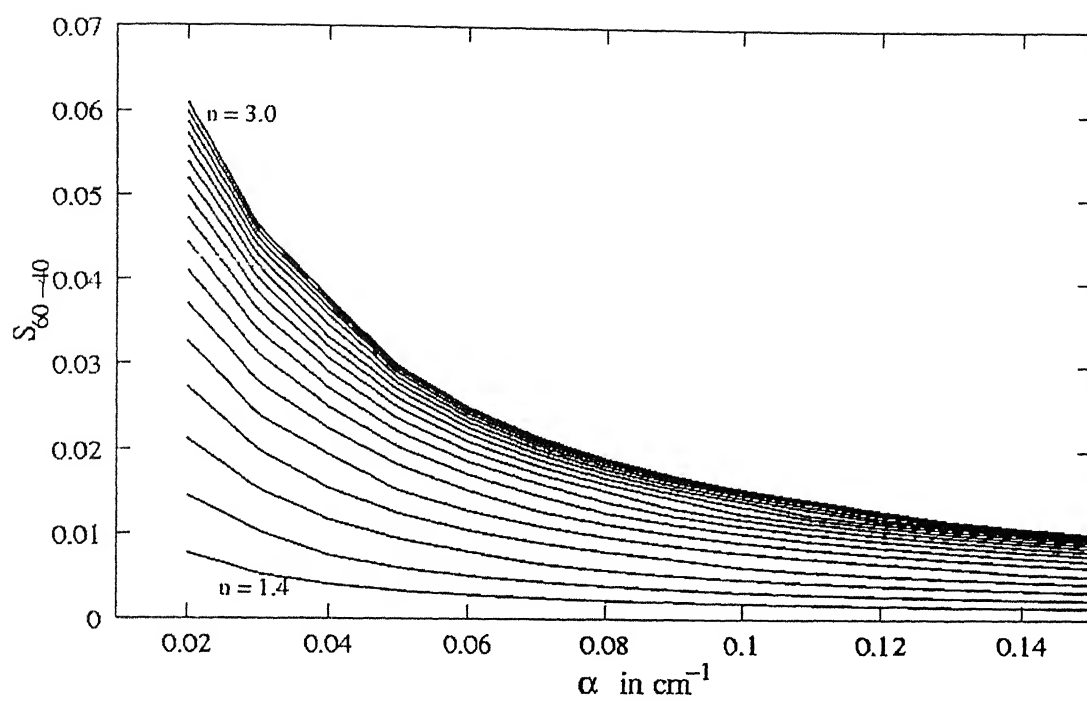


Fig. 4.7: variation of S_{60-40} with α

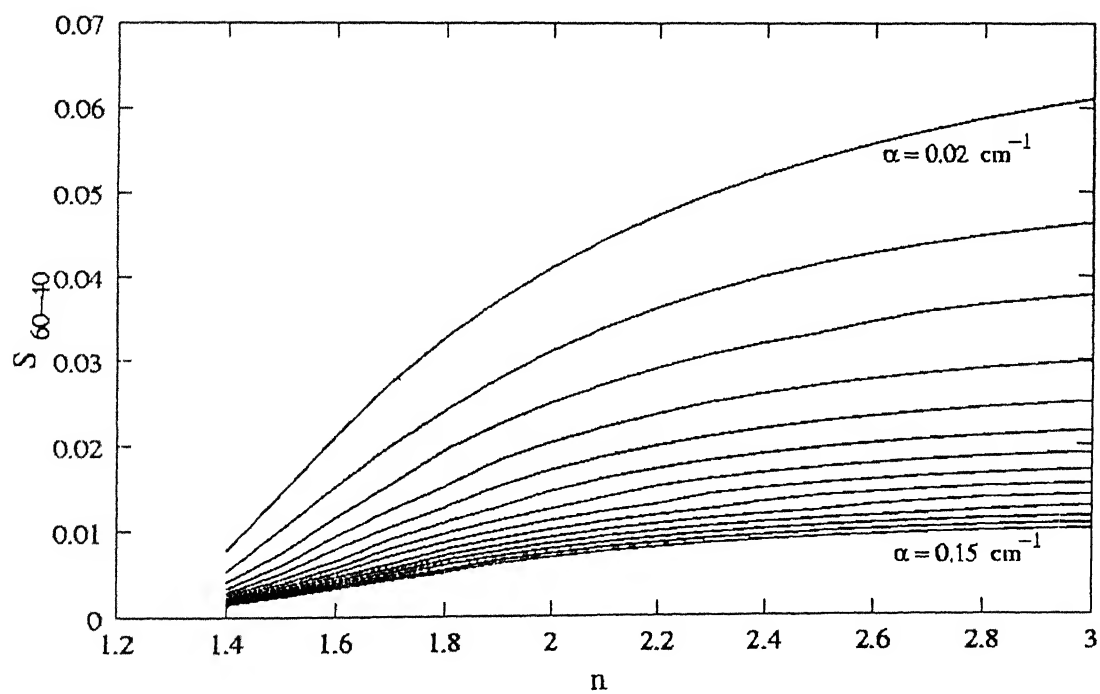


Fig. 4.8: variation of S_{60-40} with n

The various curves for S_{60-40} , obtained in fig 4.7, has been fitted in mathematical expression given in eq. (4.5) in a similar fashion as in T_{50} , if the two parameters are known.

$$T_{60} - T_{40} = T_c + A \cdot e^{-a/t} \quad (4.5)$$

where

$$T_c = -0.0117 + 0.03682 \cdot n - 0.01136 \cdot n^2 + 0.00122 \cdot n^3 \quad (4.6)$$

$$A = -0.334 + 0.41776 \cdot n - 0.1459 \cdot n^2 + 0.018 \cdot n^3 \quad (4.7)$$

and,

$$t = 0.0531 + 0.09482 \cdot n + 0.0337 \cdot n^2 + 0.0039 \cdot n^3 \quad (4.8)$$

Table 4.2 shows various values of these coefficients for various n .

Table 4.2: variation of coefficients of eq. (4.5) w.r.t. n

n	T_c	A	t
1.4	0.00158	0.0136	0.02482
1.5	0.00258	0.02543	0.02572
1.6	0.00353	0.03499	0.02844
1.7	0.00451	0.04338	0.03
1.8	0.00549	0.05061	0.03107
1.9	0.00626	0.05643	0.03229
2	0.00687	0.06151	0.03317
2.1	0.00741	0.06603	0.03369
2.2	0.00786	0.06998	0.03405
2.3	0.00828	0.07346	0.03426
2.4	0.00868	0.07673	0.03422
2.5	0.00901	0.07968	0.03415

2.6	0.00926	0.0823	0.03419
2.7	0.00946	0.08465	0.03422
2.8	0.00972	0.08698	0.03397
2.9	0.00993	0.08914	0.03371
3	0.01011	0.09112	0.03347

4.3 Relationship of T_{50} and S_{60-40} with parameters

Relationship of parameters and outflow data can be presented in two forms, graphical and mathematical. But the problem in determining mathematical form persist in the fact that this relationship will be based on the regression analysis of data obtained from the fitted equations for T_{50} and S_{60-40} [eq. (4.2) and (4.5)]. This results in increased errors of final output, i.e., estimate of parameters.

4.3.1 mathematical expression for parameters

After having equations (4.2) and (4.5) values of α and S_{60-40} can be obtained while changing T_{50} and n as independent variables. Once again repeating the similar process of curve fitting, expressions for α and n have been obtained as follows,

$$n = a + b \cdot S_{60-40} - c \cdot S_{60-40}^2 + d \cdot S_{60-40}^3 \quad (4.9)$$

where

$$a = 1.34853 - 0.47317 \cdot T_{50} + 0.74575 \cdot T_{50}^2 - 0.32916 \cdot T_{50}^3 \quad (4.10)$$

$$b = 18.5956 + 1.12316 \cdot e^{T_{50}/0.31967} \quad (4.11)$$

$$c = 417 + e^{1.4748+5.106T_{50}} \quad (4.12)$$

$$d = 1.03 \times 10^4 + e^{2.7+7.0279T_{50}} \quad (4.13)$$

Once n value is obtained, α can be estimated from eq. (4.2) as,

$$\alpha = -\frac{1}{b} \cdot \ln\left(1 - \frac{T_{50}}{a}\right) \quad (4.14)$$

where a and b can be obtained from eq. (4.3) and (4.4) respectively.

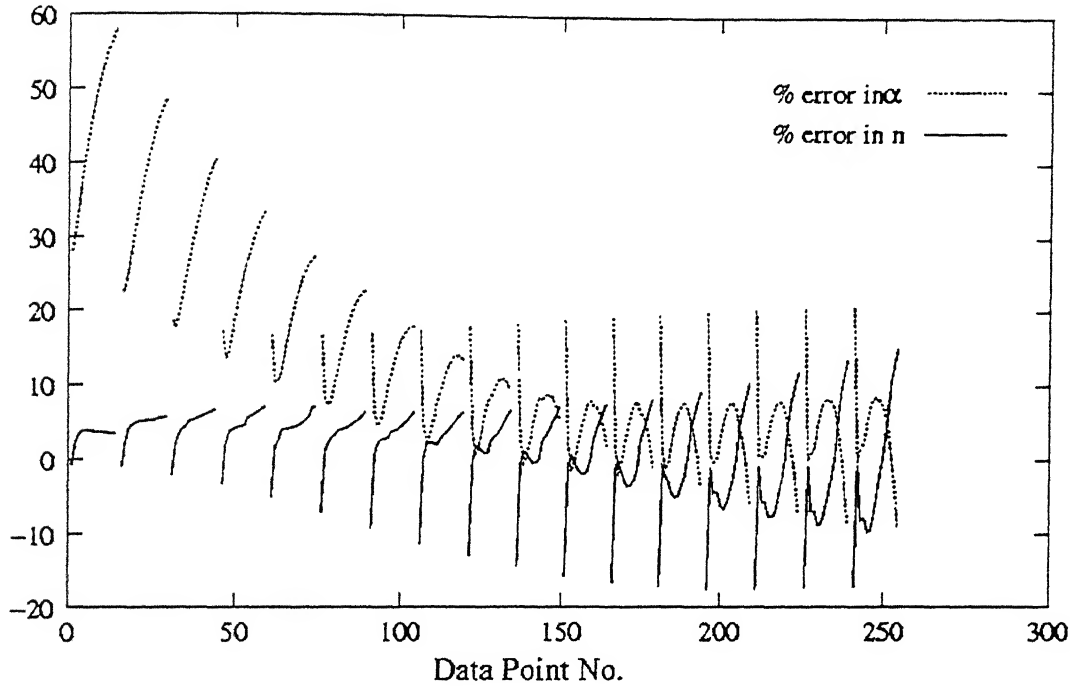


Fig. 4.9: Error in α and n back-calculated from eq (4.9) & (4.14), for 252 data sets obtained from simulation

Fig. 4.9 shows the % error in parameter estimate from eq. (4.9) and (4.14). As the errors are going beyond acceptable limits, the mathematical expression derived above, are only reliable for a very short range, $\alpha = 0.03$ to 0.14 and $n = 1.9$ to 3 . it is clear from the range that equations are valid only for coarser soils.

The main problem persist with the repeated regression, and hence the value of parameters is highly sensitive to the coefficients of eq. (4.9) and (4.14). Even a very small variation in these coefficients can severely affect the output.

4.3.2 Graphical representation of T_{50} and S_{60-40} to estimate parameters

In view of above discussion, it is clear that a well-correlated relationship can be established between outflow and flow parameters. Fig 4.9 illustrates a graphical representation of T_{50} and S_{60-40} showing the influence of parameters.

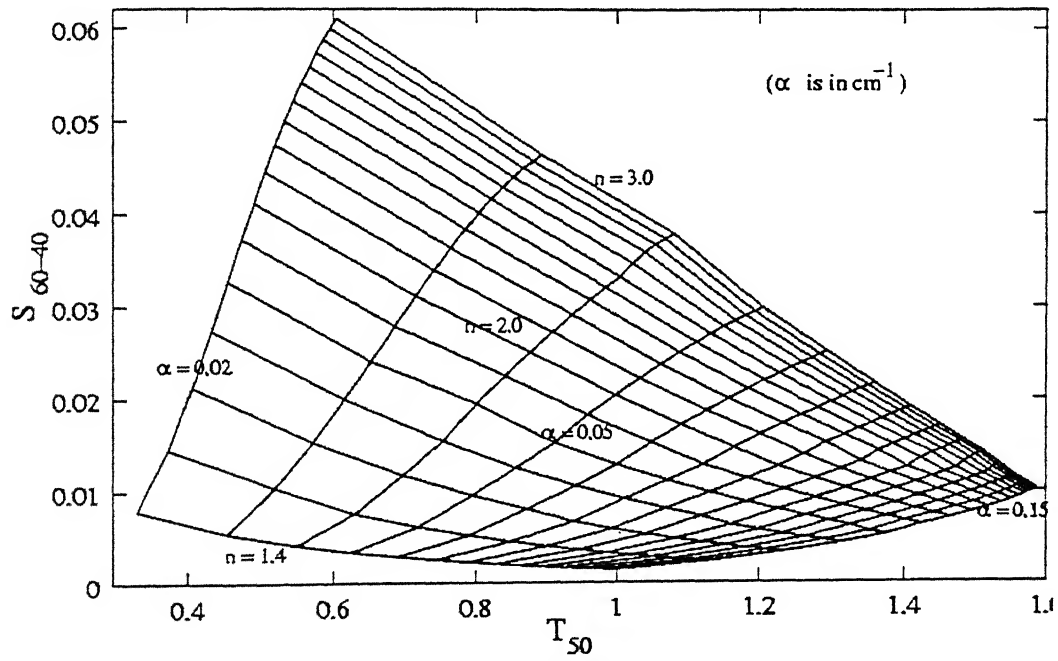


Fig. 4.10: S_{60-40} vs. T_{50} : graphical representation of studied domain of numerical values of parameters

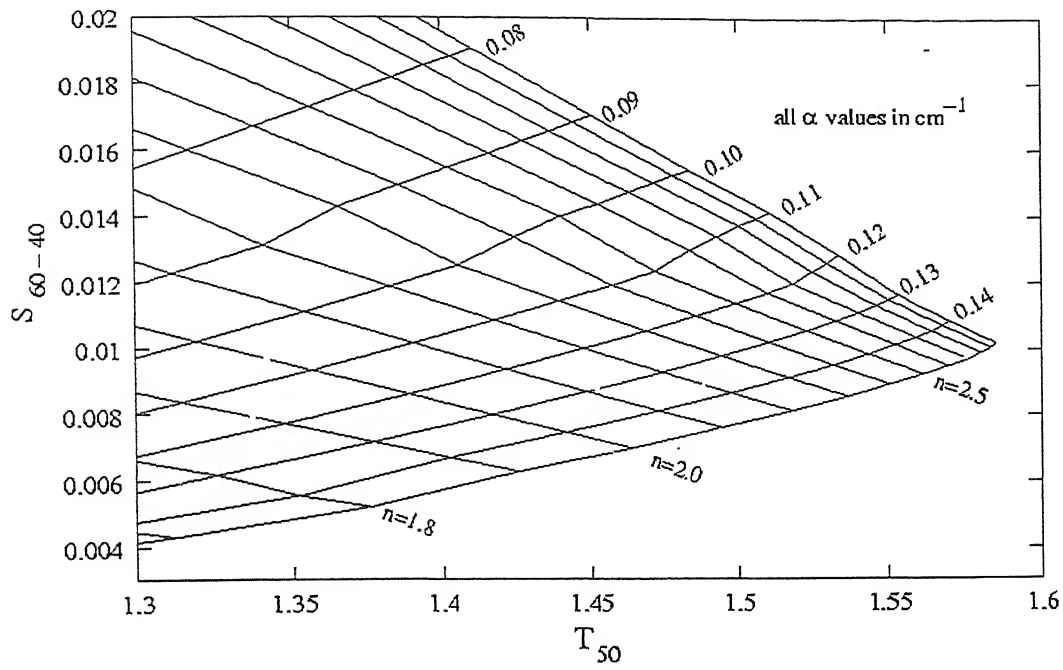


Fig. 4.11: T_{50} and S_{60-40} for higher values of α and n

This chart showing various combinations of T_{50} and S_{60-40} can easily be used for estimation of VGM parameters. At the higher values of α and n fig. 4.8 shows very congested points, hence this part is shown in fig 4.10 for convenience.

Now, using fig. (4.9) and (4.10) values of parameters can be estimated, knowing the T_{50} and S_{60-40} from outflow data.

Chapter 5

CONCLUSIONS AND FUTURE STUDY

5.1 Conclusions

The objective of this dissertation is to study the outflow in order to give a suitable method for estimation of flow parameters. As discussed in Chapter 4, the graphical representation of outflow quantities (T_{50} and S_{60-40}) is quite convenient way to get an estimate of α and n . The whole study can be concluded in following points:

- Outflow can be very smoothly correlated with the unsaturated flow parameters, by defining the two quantities, T_{50} and S_{60-40} .
- Any mathematical model is difficult to obtain for the whole range of α and n due to two reasons:
 - (1) Both parameters are highly sensitive to the input. Even for a small error in input (T_{50} and S_{60-40}) can lead to an unacceptable error in parameter estimate.
 - (2) Since the input has to be an experimental data, it cannot be expected to have perfect precision.
- A graphical representation has been given, from which the parameters can be easily estimated, knowing T_{50} and S_{60-40} .

5.2 Recommendations for future work

Present study is mainly focused on outflow data and the emphasis is on soils of sandy nature (the smaller values of α and n have not been analyzed). The phenomenon may be quite different for very small values of α and n . For smaller values of parameters ($\alpha < 0.02$ and $n < 1.4$) the convergence is very difficult to obtain. So, with the development of a better convergence scheme, the phenomenon should be studied for very small values of parameters.

The boundary condition, itself, can make significant changes in the outflow and thus in T_{50} and S_{60-40} . Hence the effect of boundary condition needs to be studied.

In the proposed method main focus is on outflow data, but the pressure head (as discussed in Chapter-4) can also be used to estimate the parameters.

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